Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2024 – 12:33 am GMT

PDB ID	:	4UN7
Title	:	THE CRYSTAL STRUCTURE OF I-DMOI IN COMPLEX WITH ITS TARGET DNA BEFORE INCUBATION IN 5MM MN (STATE 1)
Authors	:	Molina, R.; Stella, S.; Redondo, P.; Gomez, H.; Marcaida, M.J.; Orozco, M.; Prieto, J.; Montoya, G.
Deposited on	:	2014-05-26
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

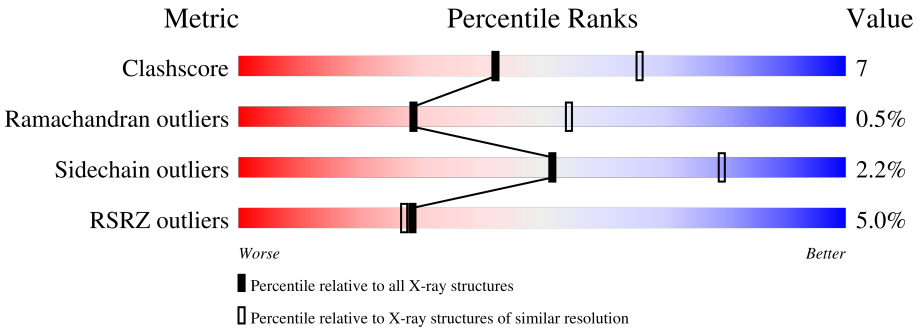
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	199	6%, 70%, 20%, 8%
1	D	199	7%, 82%, 13%
2	B	25	72%, 28%
2	E	25	60%, 40%
2	H	25	60%, 36%
3	C	25	84%, 16%

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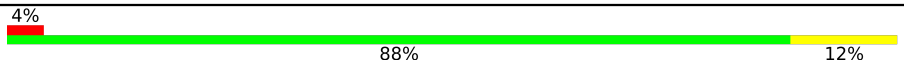
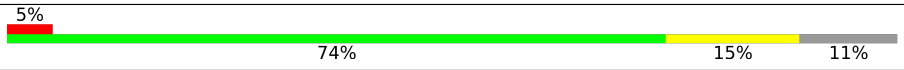
Mol	Chain	Length	Quality of chain
3	F	25	
3	I	25	
4	G	199	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7780 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called HOMING ENDONUCLEASE I-DMOI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	184	Total	C	N	O	S	0	3	0
			1541	993	282	263	3			
1	D	191	Total	C	N	O	S	0	4	0
			1596	1030	291	272	3			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	ALA	-	expression tag	UNP P21505
A	189	ALA	-	expression tag	UNP P21505
A	190	ALA	-	expression tag	UNP P21505
A	191	ALA	-	expression tag	UNP P21505
A	192	LEU	-	expression tag	UNP P21505
A	193	GLU	-	expression tag	UNP P21505
A	194	HIS	-	expression tag	UNP P21505
A	195	HIS	-	expression tag	UNP P21505
A	196	HIS	-	expression tag	UNP P21505
A	197	HIS	-	expression tag	UNP P21505
A	198	HIS	-	expression tag	UNP P21505
A	199	HIS	-	expression tag	UNP P21505
D	1	ALA	-	expression tag	UNP P21505
D	189	ALA	-	expression tag	UNP P21505
D	190	ALA	-	expression tag	UNP P21505
D	191	ALA	-	expression tag	UNP P21505
D	192	LEU	-	expression tag	UNP P21505
D	193	GLU	-	expression tag	UNP P21505
D	194	HIS	-	expression tag	UNP P21505
D	195	HIS	-	expression tag	UNP P21505
D	196	HIS	-	expression tag	UNP P21505
D	197	HIS	-	expression tag	UNP P21505
D	198	HIS	-	expression tag	UNP P21505
D	199	HIS	-	expression tag	UNP P21505

- Molecule 2 is a DNA chain called 25MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	25	Total	C	N	O	P	0	0	0
			511	242	94	151	24			
2	E	25	Total	C	N	O	P	0	0	0
			511	242	94	151	24			
2	H	25	Total	C	N	O	P	0	0	0
			511	242	94	151	24			

- Molecule 3 is a DNA chain called 25MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	25	Total	C	N	O	P	0	0	0
			508	240	99	145	24			
3	F	25	Total	C	N	O	P	0	0	0
			508	240	99	145	24			
3	I	25	Total	C	N	O	P	0	0	0
			508	240	99	145	24			

- Molecule 4 is a protein called HOMING ENDONUCLEASE I-DMOI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	177	Total	C	N	O	S	0	4	0
			1487	962	270	252	3			

There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	1	ALA	-	expression tag	UNP P21505
G	6	GLU	ASN	conflict	UNP P21505
G	189	ALA	-	expression tag	UNP P21505
G	190	ALA	-	expression tag	UNP P21505
G	191	ALA	-	expression tag	UNP P21505
G	192	LEU	-	expression tag	UNP P21505
G	193	GLU	-	expression tag	UNP P21505
G	194	HIS	-	expression tag	UNP P21505
G	195	HIS	-	expression tag	UNP P21505
G	196	HIS	-	expression tag	UNP P21505
G	197	HIS	-	expression tag	UNP P21505
G	198	HIS	-	expression tag	UNP P21505
G	199	HIS	-	expression tag	UNP P21505

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Zn 1 1	0	0
5	D	1	Total Zn 1 1	0	0
5	G	1	Total Zn 1 1	0	0

- Molecule 6 is water.

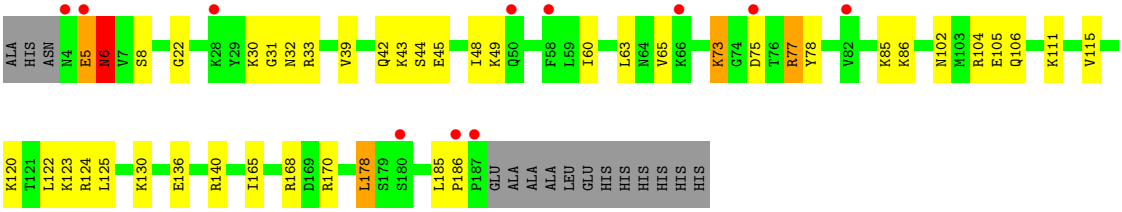
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	22	Total O 22 22	0	0
6	B	6	Total O 6 6	0	0
6	C	2	Total O 2 2	0	0
6	D	22	Total O 22 22	0	0
6	E	6	Total O 6 6	0	0
6	F	5	Total O 5 5	0	0
6	G	25	Total O 25 25	0	0
6	H	2	Total O 2 2	0	0
6	I	6	Total O 6 6	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: HOMING ENDONUCLEASE I-DMOI

Chain A:



• Molecule 1: HOMING ENDONUCLEASE I-DMOI

Chain D:

• Molecule 2: 25MER

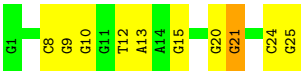
Chain B:

• Molecule 2: 25MER

Chain E:

• Molecule 2: 25MER

Chain H:

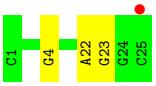


• Molecule 3: 25MER

Chain C:

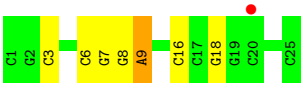
• Molecule 3: 25MER

Chain F:



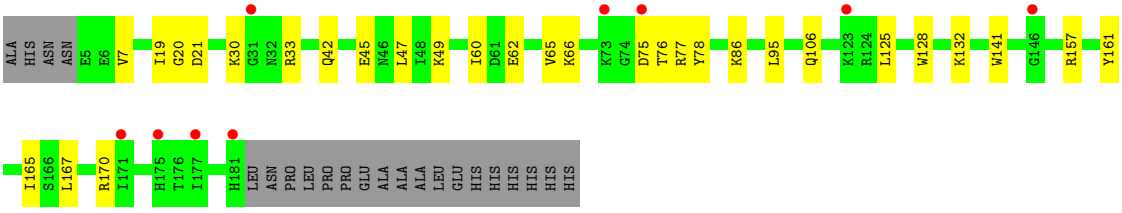
• Molecule 3: 25MER

Chain I:



• Molecule 4: HOMING ENDONUCLEASE I-DMOI

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.57Å 70.35Å 106.60Å 90.00° 119.89° 90.00°	Depositor
Resolution (Å)	46.20 – 2.70 46.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (46.20-2.70) 99.7 (46.20-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.04 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.177 , 0.232 0.186 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	68.4	Xtriage
Anisotropy	0.485	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 60.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.047 for -h-l,k,h 0.047 for l,k,-h-l 0.032 for h,-k,-h-l 0.027 for -h-l,-k,l 0.027 for l,-k,h	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	7780	wwPDB-VP
Average B, all atoms (Å^2)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.53	0/1576	0.64	0/2121
1	D	0.43	0/1640	0.59	1/2208 (0.0%)
2	B	0.97	0/572	1.06	0/882
2	E	0.88	0/572	1.03	0/882
2	H	0.92	0/572	1.02	1/882 (0.1%)
3	C	0.90	0/570	1.00	2/877 (0.2%)
3	F	0.88	0/570	0.89	0/877
3	I	0.84	0/570	1.02	3/877 (0.3%)
4	G	0.44	0/1525	0.62	0/2046
All	All	0.68	0/8167	0.82	7/11652 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	21	DG	O4'-C4'-C3'	-6.45	101.92	104.50
3	I	9	DA	O4'-C1'-N9	6.45	112.51	108.00
3	I	3	DC	C1'-O4'-C4'	-6.18	103.92	110.10
3	C	18	DG	O4'-C1'-N9	5.71	112.00	108.00
3	C	6	DC	C1'-O4'-C4'	-5.42	104.69	110.10
3	I	18	DG	O4'-C1'-N9	5.24	111.67	108.00
1	D	77	ARG	NE-CZ-NH1	5.17	122.89	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	5	GLU	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1541	0	1617	29	1
1	D	1596	0	1671	22	0
2	B	511	0	282	8	0
2	E	511	0	282	6	1
2	H	511	0	282	7	0
3	C	508	0	279	2	0
3	F	508	0	279	3	0
3	I	508	0	279	4	0
4	G	1487	0	1574	24	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
5	G	1	0	0	0	0
6	A	22	0	0	2	0
6	B	6	0	0	0	0
6	C	2	0	0	0	0
6	D	22	0	0	1	0
6	E	6	0	0	0	0
6	F	5	0	0	1	0
6	G	25	0	0	4	0
6	H	2	0	0	0	0
6	I	6	0	0	0	0
All	All	7780	0	6545	94	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (94) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:NZ	6:A:2005:HOH:O	2.04	0.91
4:G:77:ARG:HH11	4:G:77:ARG:HG3	1.39	0.88
1:D:33:ARG:NH1	2:E:21:DG:O6	2.10	0.84
1:D:21:ASP:OD2	1:D:42:GLN:NE2	2.20	0.74
4:G:42:GLN:HG2	4:G:47:LEU:HD23	1.70	0.72
4:G:45:GLU:OE2	4:G:49:LYS:NZ	2.16	0.72
1:A:63:LEU:O	1:A:86:LYS:NZ	2.25	0.68
4:G:21:ASP:OD1	6:G:2004:HOH:O	2.12	0.68
1:D:77:ARG:HG2	1:D:77:ARG:HH11	1.58	0.67
1:A:43:LYS:NZ	2:B:13:DA:OP1	2.25	0.67
1:A:77:ARG:HG2	1:A:77:ARG:HH11	1.60	0.67
1:A:30:LYS:HD2	1:A:31:GLY:H	1.62	0.65
4:G:33:ARG:NH1	2:H:21:DG:O6	2.30	0.64
4:G:20:GLY:O	6:G:2002:HOH:O	2.15	0.63
1:D:43:LYS:HE2	2:E:13:DA:OP2	1.98	0.62
4:G:30:LYS:NZ	2:H:20:DG:OP2	2.33	0.62
3:I:6:DC:H2"	3:I:7:DG:H5'	1.81	0.62
1:A:31:GLY:HA3	1:A:33:ARG:HG3	1.82	0.61
1:A:60:ILE:HG23	1:A:65:VAL:HB	1.86	0.58
1:A:73:LYS:HD2	1:A:78:TYR:HE1	1.70	0.57
1:A:45:GLU:HB2	1:A:78:TYR:CE2	2.40	0.57
2:H:24:DC:H2'	2:H:25:DG:C8	2.40	0.56
1:D:77:ARG:HH11	1:D:77:ARG:CG	2.19	0.56
4:G:45:GLU:HB2	4:G:78:TYR:CE2	2.41	0.55
2:B:5:DT:H2"	2:B:6:DG:C8	2.42	0.54
1:D:111:LYS:HD2	1:D:186:PRO:HD3	1.88	0.54
1:D:30:LYS:N	1:D:30:LYS:HD3	2.23	0.54
4:G:19:ILE:HD11	4:G:95:LEU:HD13	1.90	0.54
1:A:115:VAL:O	1:A:120:LYS:NZ	2.23	0.53
4:G:77:ARG:HG3	4:G:77:ARG:NH1	2.09	0.53
1:D:136:GLU:O	1:D:140:ARG:HG3	2.09	0.52
4:G:170:ARG:NH1	6:G:2025:HOH:O	2.28	0.52
1:A:42:GLN:HG2	6:A:2010:HOH:O	2.09	0.51
1:D:21:ASP:OD1	6:D:2002:HOH:O	2.19	0.51
1:D:125:LEU:HB2	1:D:165:ILE:HB	1.92	0.51
2:E:8:DC:H2"	2:E:9:DG:C8	2.46	0.50
2:E:19:DC:H2'	2:E:20:DG:C8	2.47	0.50
1:A:111:LYS:O	1:A:115:VAL:HG23	2.12	0.48
1:A:30:LYS:HD2	1:A:31:GLY:N	2.27	0.48
1:D:97:ARG:HB2	1:D:100:LEU:HD12	1.96	0.48
1:D:111:LYS:HD2	1:D:186:PRO:CD	2.45	0.47
1:A:102:ASN:O	1:A:106:GLN:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:25:DG:OP2	4:G:86:LYS:HE3	2.14	0.47
1:A:122:LEU:HB2	1:A:186:PRO:HG3	1.97	0.47
3:F:22:DA:H2"	3:F:23:DG:C8	2.50	0.47
1:A:136:GLU:O	1:A:140:ARG:HG3	2.15	0.47
1:D:45:GLU:OE2	1:D:49:LYS:HE3	2.14	0.46
4:G:125:LEU:HB2	4:G:165:ILE:HB	1.97	0.46
4:G:60:ILE:HG23	4:G:65:VAL:HB	1.98	0.46
4:G:128:TRP:CZ3	3:I:16:DC:H2'	2.50	0.46
1:A:31:GLY:HA3	1:A:33:ARG:H	1.80	0.46
1:A:45:GLU:HG3	1:A:49:LYS:HE3	1.98	0.46
1:A:130:LYS:HG3	3:C:15:DC:OP2	2.16	0.45
2:E:5:DT:H2"	2:E:6:DG:C8	2.51	0.45
2:E:11:DG:H2"	2:E:12:DT:H71	1.98	0.45
1:A:85:LYS:NZ	3:C:4:DG:OP1	2.40	0.45
4:G:132:LYS:HD2	4:G:161:TYR:CZ	2.51	0.45
1:A:123:LYS:O	1:A:170:ARG:NH2	2.49	0.45
1:D:5:GLU:O	1:D:6:ASN:HB3	2.16	0.45
1:D:185:LEU:HA	1:D:186:PRO:HD2	1.76	0.44
1:A:178:LEU:HD23	1:A:178:LEU:HA	1.85	0.44
1:D:33:ARG:HD2	3:F:4:DG:O6	2.17	0.44
2:B:19:DC:H2'	2:B:20:DG:C8	2.53	0.44
2:B:5:DT:H2"	2:B:6:DG:H8	1.81	0.43
2:B:6:DG:H1'	2:B:7:DC:H5"	1.99	0.43
3:I:8:DG:H2"	3:I:9:DA:H5'	1.99	0.43
2:H:8:DC:H2"	2:H:9:DG:C8	2.54	0.43
3:F:22:DA:H2"	3:F:23:DG:H8	1.84	0.43
3:I:7:DG:H2"	3:I:8:DG:H5"	2.00	0.43
2:B:6:DG:H2"	2:B:7:DC:H5'	2.01	0.43
1:D:65:VAL:HG22	1:D:86:LYS:HD3	2.01	0.43
4:G:77:ARG:NE	2:H:15:DG:N7	2.67	0.43
4:G:106:GLN:HG2	4:G:141:TRP:CD2	2.54	0.43
1:A:125:LEU:HB2	1:A:165:ILE:HB	2.01	0.42
4:G:167:LEU:HD23	4:G:167:LEU:HA	1.81	0.42
1:D:170:ARG:HG2	1:D:171:ILE:HD12	2.00	0.42
1:A:22:GLY:HA3	1:A:39:VAL:O	2.20	0.42
1:A:170:ARG:HD3	1:A:185:LEU:HG	2.01	0.42
4:G:75:ASP:OD1	4:G:76:THR:N	2.52	0.42
1:A:77:ARG:HG2	1:A:77:ARG:NH1	2.33	0.42
4:G:157:ARG:NH2	2:H:10:DG:O6	2.40	0.42
1:D:77:ARG:HG2	1:D:77:ARG:O	2.20	0.41
4:G:7:VAL:HG21	4:G:62:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HA	1:A:186:PRO:HD2	1.95	0.41
2:H:12:DT:H2"	2:H:13:DA:C8	2.56	0.41
1:D:120:LYS:HE2	6:F:2004:HOH:O	2.19	0.41
4:G:106:GLN:HG2	4:G:141:TRP:CE2	2.56	0.41
1:D:47:LEU:HD12	1:D:51:HIS:HB3	2.02	0.40
4:G:132:LYS:HD2	4:G:161:TYR:CE2	2.56	0.40
1:A:8:SER:HB2	1:A:105:GLU:OE2	2.21	0.40
1:D:186:PRO:HA	1:D:187:PRO:HD3	1.92	0.40
1:A:5:GLU:HG2	1:A:6:ASN:H	1.86	0.40
2:B:19:DC:H2"	2:B:20:DG:H5'	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:ARG:NH2	2:E:19:DC:OP1[2_555]	2.06	0.14

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	185/199 (93%)	175 (95%)	7 (4%)	3 (2%)	9 24
1	D	193/199 (97%)	188 (97%)	5 (3%)	0	100 100
4	G	179/199 (90%)	175 (98%)	4 (2%)	0	100 100
All	All	557/597 (93%)	538 (97%)	16 (3%)	3 (0%)	29 54

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	178	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	170/178 (96%)	161 (95%)	9 (5%)	22 48
1	D	175/178 (98%)	173 (99%)	2 (1%)	73 90
4	G	163/178 (92%)	161 (99%)	2 (1%)	71 88
All	All	508/534 (95%)	495 (97%)	13 (3%)	52 75

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASN
1	A	44	SER
1	A	48	ILE
1	A	73	LYS
1	A	75	ASP
1	A	77	ARG
1	A	124	ARG
1	A	168[A]	ARG
1	A	168[B]	ARG
1	D	30	LYS
1	D	77	ARG
4	G	66[A]	LYS
4	G	66[B]	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
4	G	181	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	184/199 (92%)	0.73	11 (5%)	21	20	42, 60, 103, 136	0
1	D	191/199 (95%)	0.69	13 (6%)	17	15	40, 61, 96, 123	0
2	B	25/25 (100%)	-0.26	0	100	100	50, 66, 78, 81	0
2	E	25/25 (100%)	0.12	0	100	100	49, 71, 93, 96	0
2	H	25/25 (100%)	0.20	0	100	100	51, 65, 83, 90	0
3	C	25/25 (100%)	-0.10	0	100	100	50, 67, 84, 86	0
3	F	25/25 (100%)	0.36	1 (4%)	38	37	50, 64, 104, 115	0
3	I	25/25 (100%)	0.47	1 (4%)	38	37	46, 65, 99, 102	0
4	G	177/199 (88%)	0.61	9 (5%)	28	26	39, 54, 80, 129	0
All	All	702/747 (93%)	0.56	35 (4%)	28	27	39, 61, 95, 136	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	187	PRO	4.8
1	D	195	HIS	4.2
1	D	192	LEU	3.9
1	D	182	LEU	3.7
1	A	186	PRO	3.7
1	D	191	ALA	3.4
1	D	168	ARG	3.2
1	D	188	GLU	3.2
1	A	5	GLU	3.0
4	G	181	HIS	2.9
4	G	73	LYS	2.9
4	G	177	ILE	2.8
4	G	75	ASP	2.6
1	D	177	ILE	2.6
4	G	123	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	181	HIS	2.6
3	I	20	DC	2.5
1	A	75	ASP	2.5
4	G	175	HIS	2.4
1	D	140	ARG	2.4
1	A	28	LYS	2.4
1	D	30	LYS	2.3
4	G	146	GLY	2.3
1	A	4	ASN	2.3
1	D	194	HIS	2.2
1	A	66	LYS	2.2
1	D	144	ASN	2.2
4	G	171	ILE	2.2
1	A	180	SER	2.1
1	A	58	PHE	2.1
1	A	50	GLN	2.1
1	A	82	VAL	2.1
4	G	31	GLY	2.1
3	F	25	DC	2.1
1	D	187	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ZN	D	1197	1/1	0.97	0.12	80,80,80,80	0
5	ZN	A	1188	1/1	0.98	0.10	87,87,87,87	0
5	ZN	G	1182	1/1	0.99	0.08	88,88,88,88	0

6.5 Other polymers (i)

There are no such residues in this entry.